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NASA Technical Memorandum 105731
AIAA–92–3338

Applied Analytical Combustion/Emissions Research at the NASA Lewis Research Center: A Progress Report

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July 1992

NASA

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Abstract

Emissions of pollutants from future commercial transports are a significant concern. As a result, the Lewis Research Center (LeRC) is investigating various low emissions combustor technologies. As part of this effort, a combustor analysis code development program has been pursued to guide the combustor design process, to identify concepts having the greatest promise, and to optimize them at the lowest cost in the minimum time.

Introduction

The LeRC analytical research program is being conducted over a period of five years and involves three milestones: The first, already completed, involved development and application of 2-D and 3-D codes to guide combustion concept experiments. Second, these codes will be updated by the end of FY93 using results obtained from combustion concept experiments. Finally, these codes will be employed by the end of FY95 as predictive design tools for low emissions combustors.[1]

Due to the complexity and scope of this effort, work has been divided between numerous researchers at several sites, as shown in Figure 1. These researchers are employing a variety of tools including KIVA-II and LeRC-3D, computational fluid dynamics (CFD) codes for multi-dimensional analyses of reacting flows, and LSENS, a general chemical kinetics code for one-dimensional studies:

- KIVA-II is an advanced, widely used multi-dimensional CFD program for the prediction of the in-cylinder combustion dynamics of internal combustion engines. Because the code is well-suited for problems combining sprays, turbulence, and combustion, it has been modified to analyze gas turbine combustors.[2]
- LeRC-3D was also devised to study turbulent reacting flows with sprays in internal combustion engines. Like KIVA-II, this advanced code has been modified for studies of gas turbine combustors.[3]
- Because of its computational speed, LSENS is useful in the development and testing of reduced kinetics mechanisms needed by the CFD codes.[4]

Key features of all three codes are summarized in Table 1.

KIVA-II Combustor Analyses

In the past year, KIVA-II has been successfully applied to analyze various combustor concepts, including Lean Premixed Prevaporized (LPP) and Rich Burn/Quick Mix/Lean Burn (RQL) designs, with favorable comparisons to experimental data available in the literature.

LPP Flame Tube Analyses

A generic LPP flame tube is shown in Figure 2. The high temperature section of this device consists of an inlet section, fuel injector, vaporization section, flameholder, and combustion section.[5,6]

LPP Vaporization Analysis

To provide a uniform fuel/air mixture to the combustion section, vaporization of the injected liquid fuel, e.g., Jet-A, and mixing of the vaporized fuel with air must be completed upstream of the flameholder. Since inlet conditions control the degree to which this can be accomplished, they must be chosen carefully; however, because of the number of variables involved, it is often difficult to do so a priori. To identify the relationships between the inflow parameters, a three-

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dimensional sector analysis of the spray vaporization process in a typical LPP injector venturi has been developed using KIVA-II.

In the course of developing this analysis, it was found that convergence was hampered by lightly damped downstream oscillations in flow properties. Using an averaging scheme based on the pressure in a specified downstream cell, KIVA-II has been modified to time average the solution to increase the damping and speed convergence to the steady state.[7]

Some preliminary results are shown in Figure 3, where droplet population contour maps for the centerline plane of the venturi are provided for two sets of inflow conditions. As expected, vaporization is completed much more quickly as the inlet temperature is increased.

More detailed comparisons to experimental data and further parametric studies are anticipated in the near future.

LPP Combustion Analysis

Analysis of the combustion in an LPP flame tube is complicated by the flowfield in the vicinity of the flameholder. In order to accurately model the combustion process, a representation of the flameholder is required.

Unfortunately, in its original form, KIVA-II cannot describe an inflow boundary with the complicated geometry typically seen in the flameholders used in these combustors. However, owing to its piston engine origins, KIVA-II does incorporate a scheme to input a complicated cylinder head geometry. Since the cylinder head is used represent the inflow boundary in flame tube calculations, the existing coding which describes the cylinder head geometry was selected to also describe the flameholder geometry. Although some initial difficulties were encountered in modifying the application of the upstream boundary condition to specify which cells along the head were open or closed, these have been resolved.[7]

Figure 4 shows the geometry of a typical flameholder, while Figure 5 displays the grid used in the corresponding KIVA-II analysis. To reduce the computational burden, the two-dimensional array of holes has been represented by annular rings to allow an axisymmetric analysis to be performed. To maintain a similar flow pattern, the width of the annuli and the spacing between them have been chosen to approximate the hole diameters and spacing. By adopting this approach, one problem is created in that the flow blockage due to the flameholder will be underestimated. Future studies will address the significance of this assumption.

In examining the combustion process in the LPP flame tube, the principal interest is the emissions of pollutants such as nitrogen oxides, NO_x. However, even the LPP combustor problem is sufficiently complex to prohibit the use of detailed reaction kinetics. To maintain tractability, a reduced kinetics mechanism for propane combustion (discussed in a previous paper by the first and second authors) is employed. With 21 reaction steps involving 17 species, this mechanism has been specifically designed to provide predictions of both thermal and prompt NO_x over a wide range of equivalence ratios and initial conditions. As shown in Figure 6, reasonable agreement with available experimental data can be achieved.[8]

While these results are promising, caution must be expressed that detailed quantitative comparisons should not to be expected in general because of the complexity of even the LPP problem. Although an LPP combustor is a relatively simple device, there are numerous boundary condition problems to be addressed, and the treatment of some of these is the subject of ongoing research at LeRC.

For example, the above analysis assumes that the wall boundaries are adiabatic. Current research at LeRC aims to incorporate an explicit model to describe the details of the heat transfer between the gas within the combustor and the chamber walls.

Further, KIVA-II currently incorporates laminar kinetics to describe the combustion process, which may not be appropriate in the presence of turbulence. Again at LeRC, a model for the combustion-turbulence interaction will be incorporated into KIVA-II in the near future.

RQL Flame Tube Analyses

As shown in Figure 7, the RQL combustor is substantially more complicated than the LPP concept. As a result, the analyses performed to date have had to focus more on the fluid dynamics of the flowfield than on the chemistry of pollutant formation. In doing so, they have uncovered many details of the complicated mixing processes induced by the airblast injector and quick quench mixer.

Even more so than with the LPP burner, the RQL analysis is driven by the need to minimize the computational burden. Due to symmetry, the rich burn section can be treated with a two-dimensional analysis. However, with the crossflow jets, the mixer and lean burn sections require a three-dimensional section analysis. To minimize the overall computational time, the obvious solution is to split the combustor into two computational zones, one for the rich burn section and one for the mixer and lean burn sections. To minimize the impact of the separation of the burner on the overall solution, the computational domains for the two section contain considerable overlap.[9,10]

Because of KIVA-II's origins, the default geometry for the computational grid is cylindrical. In order to accommodate more general combustor geometries, such as that of the RQL, KIVA-II has been modified to accept an arbitrary wall geometry and to read grid information from a separate input file.[9]

For the RQL problem, advanced grid generation techniques are employed to create the computational meshes for both combustor sections:

- In the rich burn section, an algebraic/elliptic grid generator has been employed. When applied to geometries with sharp corners, as seen in an airblast injector, elliptic grid generators create poor, non-uniform grids as the grid lines tend to merge at convex corners and pull away at concave corners. However, a more uniform grid can be formed if an algebraic grid generator is used in conjunction with the elliptic generator in these regions. The success of this approach can be seen in Figure 8 which shows a grid for a generic rich burn section produced by this technique.[11]

- In the mixer region, the presence of the inclined slots complicates the development of a sector grid, since it would not be desirable to have the grid cut through one or more of the slots. By employing a three-dimensional extension of the two-dimensional transfinite interpolation technique, a twisted grid encompassing a single contiguous slot can be generated, as shown in Figure 9.[9]

Even with the combustor split to reduce computational costs, the complexity of the RQL problem still requires the use of a minimal kinetics scheme. To date, all calculations have been performed with a simple propane mechanism involving five finite rate and six equilibrium reactions, making use of KIVA-II's ability to employ finite rate kinetics for slow reactions while assuming that the fast reactions are in equilibrium. A propane mechanism is used since, for convenience, it is assumed that Jet-A vaporizes to propane.[2,9,10,12]

Results of a typical KIVA-II analysis of an RQL flame tube are shown in Figures 10 through 13. Figures 10 and 11 provide the temperature and NO_x emission index contours within the rich burn section, while Figures 12 and 13 show the same quantities for the quick quench mixer and lean burn sections.

The KIVA-II analysis for the RQL has been and continues to be used to examine various combinations of geometry configurations and inflow conditions and their impact on the emissions generated by the combustion process. Indeed, KIVA-II has become a useful diagnostic tool: published experimental results have shown that excessive coking around the airblast injectors in the rich burn section can occur. KIVA-II calculations have demonstrated that, due to the combination of inflow rates, fuel can pool in the vicinity of the injectors, explaining the coking.[9,10,13,14,15]

Enhancements to KIVA-II and LeRC-3D

Under the current project, both KIVA-II and LeRC-3D are being modified to improve their physical models and flexibility in treating complex geometries.

Although more efficient, the split analysis of the RQL introduces some uncertainty with regards to the true interaction between the rich and quick quench/lean burn sections. To provide some insight into this interaction, an analysis based on a integral, three-dimensional sector grid for the entire burner is being developed. Obviously, such a model cannot incorporate the level of complexity possible in the split analysis, so initial calculations have eliminated the airblast injector and spray vaporization aspects of the rich burn section by adopting a simpler premixed, prevaporized inflow of propane and air. Figure 14 shows the temperature distribution through a cross section of the burner for this case.[16]

Similarly, the very simple kinetics mechanism currently used to describe combustion within the RQL flame tube does not adequately treat the formation of NO_x, since it accounts for thermal, but not prompt NO_x. In the rich burn zone, prompt NO_x formation may be significant. Because of this, work continues on reducing the 21 step mechanism employed in the LPP analyses even further to facilitate use in analyses of more complicated problems, like that of the RQL burner.[8]

In this regard, KIVA-II employs an explicit sequential procedure for treating the changes in chemical composition due to each chemical reaction provided for a given problem. Because of this, the order in which the reactions are read into the program can affect the final results. This is particularly true if the major heat release is split between several steps. As more complicated kinetics mechanisms are contemplated for use with KIVA-II, this shortcoming may become significant. Because of this, KIVA-II has been modified to incorporate the CREK chemistry routine, which couples all of the reactions together, including both the finite rate and equilibrium steps.[7,17]

In addition to the conventional treatment of reaction kinetics, another approach is also being pursued at LeRC. By developing an algebraic representation of the differential equations describing the chemical kinetics, detailed mechanisms can be employed since much of the computational burden is eliminated. This research is at a very early early stage of development.[18]

Because LeRC-3D is also at an earlier stage of development, most of the work with that code in the past year has focused on completion and improvement of the basic code. In particular:

- The spray model of Raju and Sirignano previously employed in LeRC-3D has been replaced by a new implicit algorithm that promises to improve overall efficiency.[13]

- Implicit boundary conditions have been added to the LU algorithm used as the numerical flow solver.[3]

- Two schemes based on the Newton-Raphson iteration have been incorporated to improve the codes efficiency when used for problems where only a steady-state solution is desired. The first technique employs a point iterative process, while the second uses a line iterative process.[3]

Although some simple combustion problems have been analyzed with LeRC-3D, most calculations have dealt with cold flow verification of the numerical methodology, as shown in Figure 15.

Summary

The complexity of the combustor analysis problem still taxes the available computer technology. As a consequence, the degree of sophistication that can be incorporated, e.g., the kinetics, and the number of parametric studies that can be conducted are limited. Further, there are deficiencies in the models available for some key physical processes, e.g., the combustion-turbulence interaction, which can adversely affect the fidelity of the analysis.

However, even with these limitations, KIVA-II and LeRC-3D have already proved to be useful adjuncts to the experimental research program at the Lewis Research Center, and the modifications and enhancements described here have further increased their utility in the study of low emissions combustors.

As more experimental data becomes available, further deficiencies will undoubtedly be uncovered, requiring further refinements to these codes.

Acknowledgements

The authors would like to thank the researchers involved in the LeRC applied analytical combustion/emissions research program: Dr. Mike Cline (Los Alamos National Laboratory), Prof. Jerry Micklow (University of Florida), Prof. Juan Ramos (Carnegie-Mellon University), Prof. Tom Shih (Carnegie-Mellon University), Prof. Nick Winowich (University of Florida), Prof. Jason Yang (Michigan Technological University), and Prof. Ben Ying (University of South Florida).

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Table 1. Features of KIVA-II, LeRC-3D, and LSENS.[1,3,4]

KIVA-II	LeRC-3D	LSENS
■ Compressible flow	■ Compressible flow	■ Incompressible flow
■ k-ϵ turbulence model with wall functions or Sub-Grid Scale turbulence model	■ k-ϵ turbulence model with wall functions or low Re k-ϵ turbulence model (Chen and Patel)	■ Ignition and combustion in batch systems or 1-D frictionless, laminar flow
■ Laminar kinetics for arbitrary reaction mechanism with quasi-equilibrium option (mixing controlled combustion model available)	■ Laminar kinetics for two-step global reaction mechanism or mixing controlled combustion model (Magnussen and Hjertager)	■ Laminar kinetics for arbitrary finite rate reaction mechanism (global reaction treatment available)
■ Stochastic spray model with vaporization, aerodynamic breakup, turbulent dispersion, and collision sub-models	■ Non-iterative implicit spray model or explicit spray model (Raju and Sirignano)	■ Sensitivity analysis available to determine relative importance of individual reaction steps
■ Adiabatic or constant temperature wall boundaries	■ Adiabatic or constant temperature wall boundaries	■ Adiabatic and non-adiabatic boundary conditions
■ Numerical method:	■ Numerical method:	■ Numerical method:
■ 2- or 3-D time dependent finite difference code	■ Algebraic grid generator with transfinite interpolation	■ Implicit integration technique for solving stiff equations
■ Arbitrary mesh	■ Rapid convergence	■ Rapid solutions
■ ICE method with conjugate residual iteration	■ Finite volume LU or Newton-Raphson algorithm	
■ Optimal quasi-second order upwind convection	■ 1st or 2nd order accurate upwind convection	

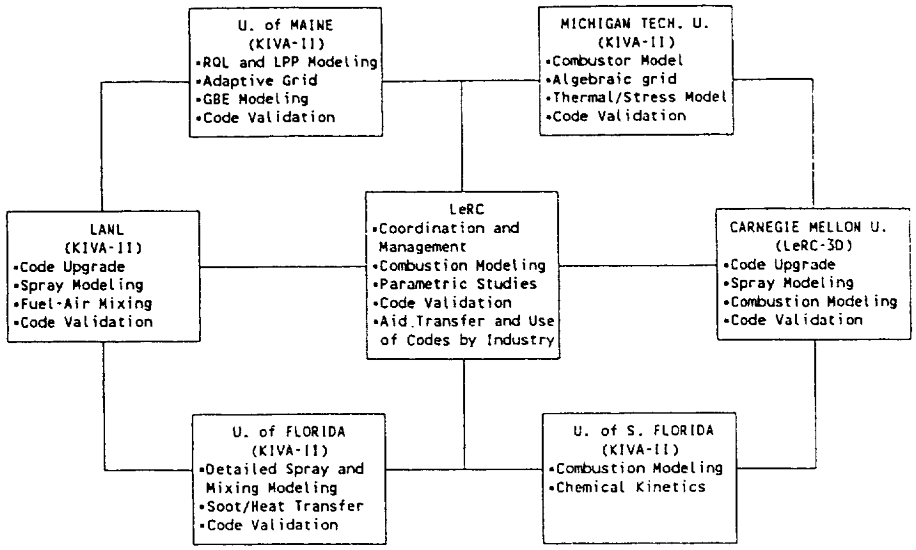

Figure 1. Applied Analytical Combustion/Emissions Research Team.

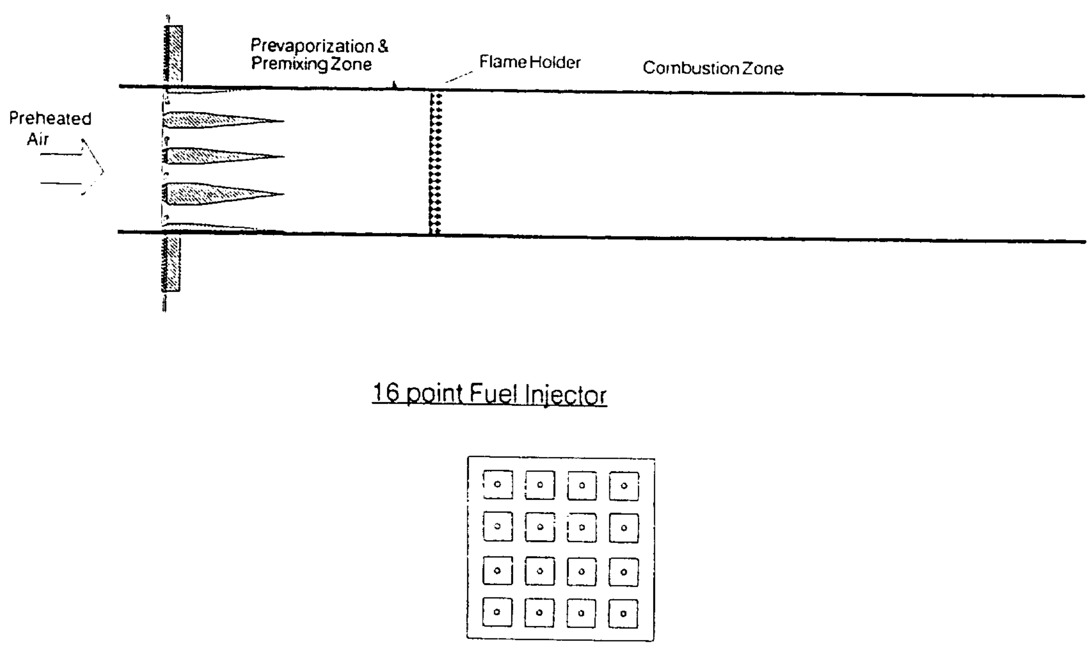

Figure 2. Generic LPP Flame Tube.[6]

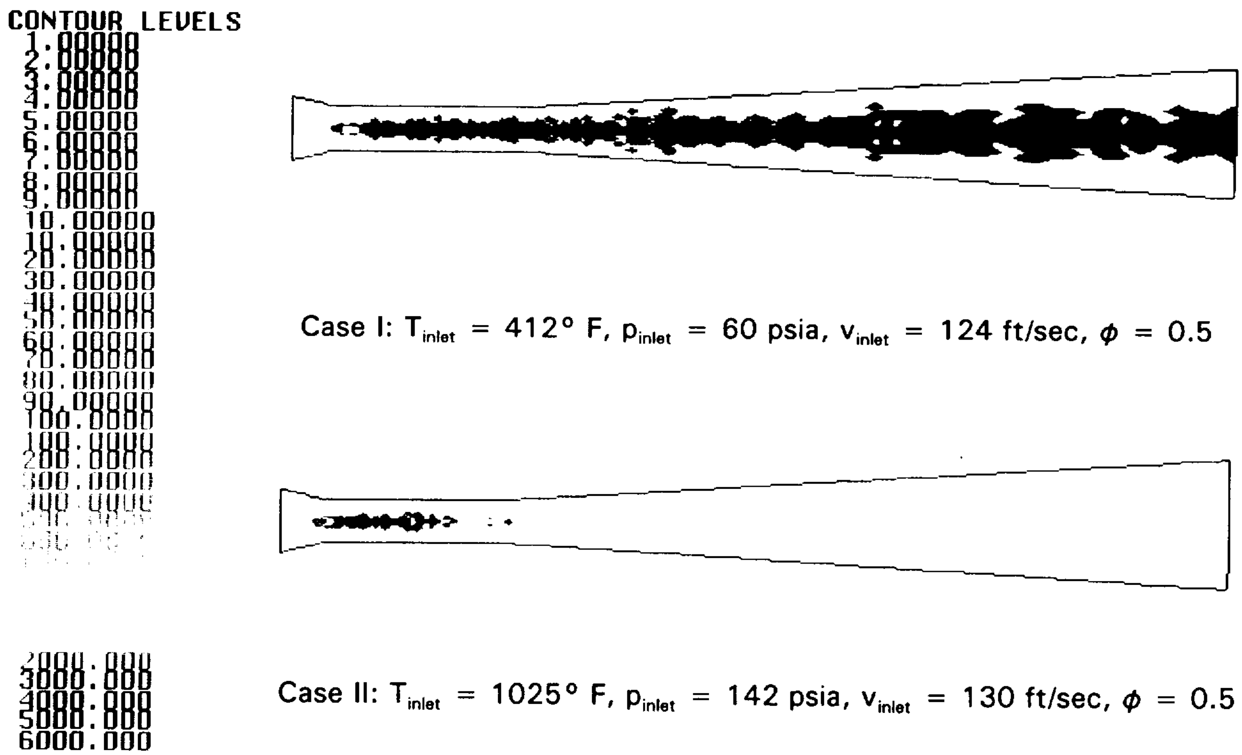

Figure 3. Jet-A Droplet Population Contours for LPP Fuel Injector Venturi.

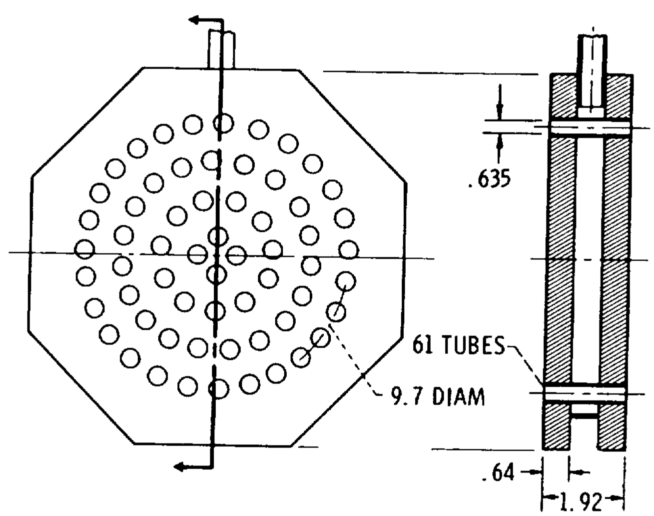

Figure 4. Flame Holder for Anderson LPP Flame Tube (Dimensions in cm).[5]

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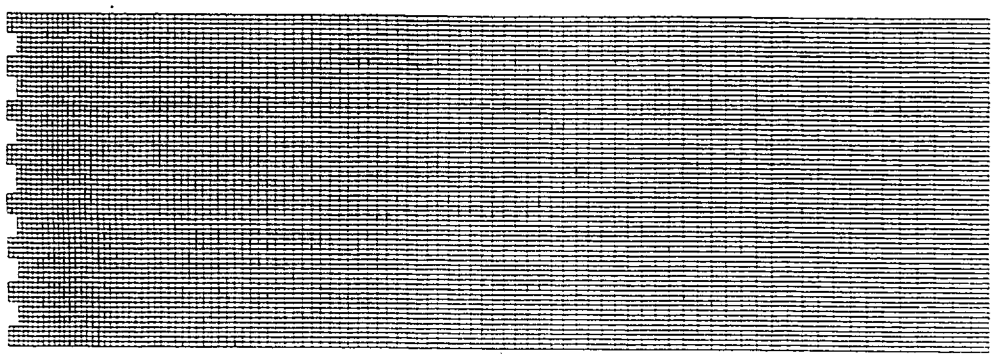

Figure 5. KIVA-II Grid for Anderson LPP Flame Tube.

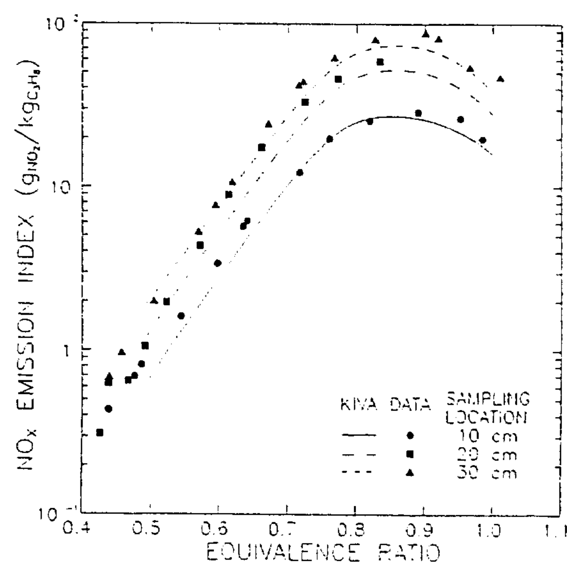

Figure 6. NO_x Emissions Comparison for Anderson LPP Flame Tube.

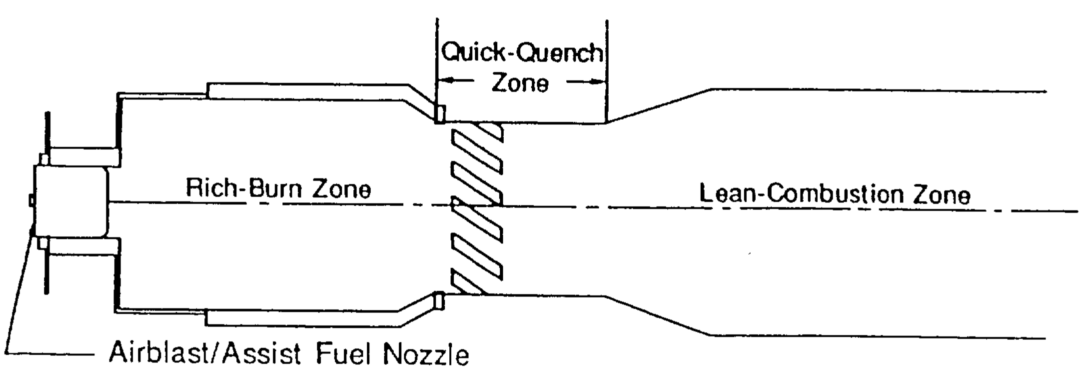

Figure 7. Generic Rich Burn - Quick Quench - Lean Burn (RQL) Flame Tube.[9]

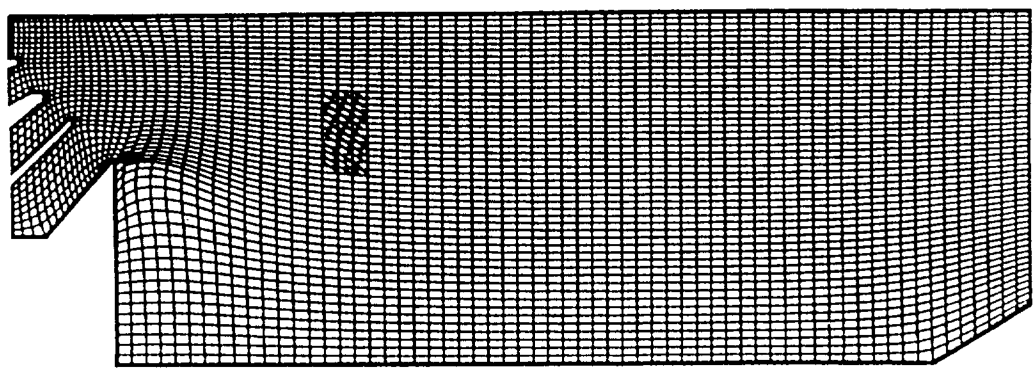

Figure 8. KIVA-II Grid for RQL Rich Burn Section.[9]

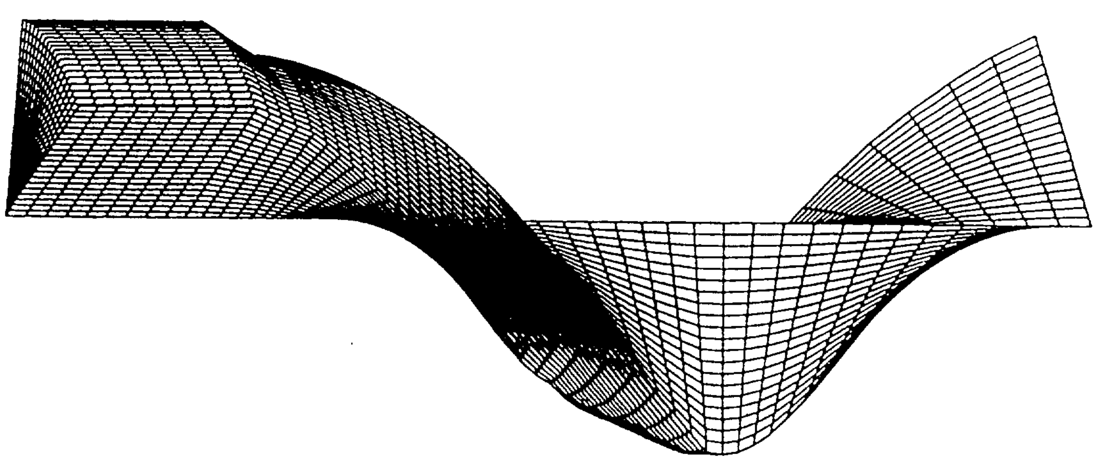

Figure 9. KIVA-II Grid for RQL Quick Quench - Lean Burn Section.[9]

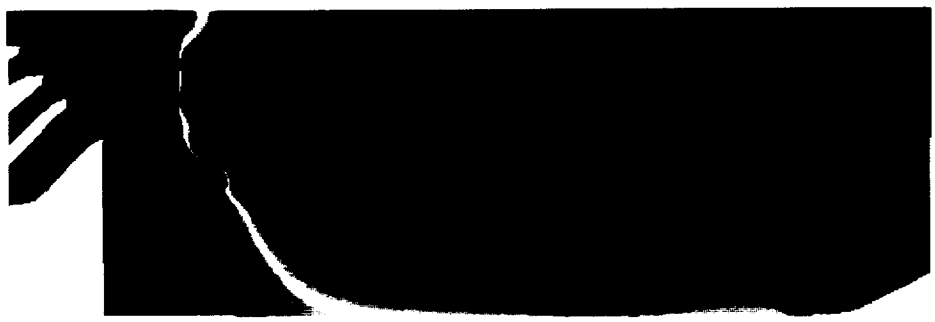

Figure 10. Temperature Contours for RQL Rich Burn Section.

Figure 11. NO_x Emissions Contours for RQL Rich Burn Section.

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Figure 12. Temperature Contours for RQL Quick Quench - Lean Burn Section.

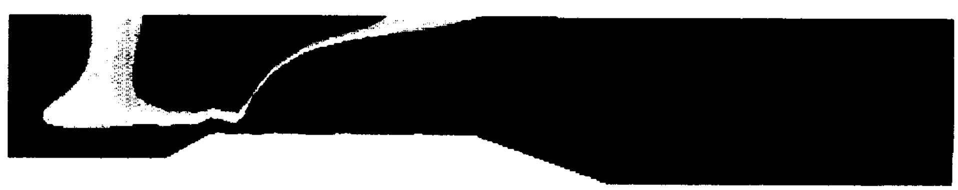

Figure 13. NO_x Emissions Contours for RQL Quick Quench - Lean Burn Section.

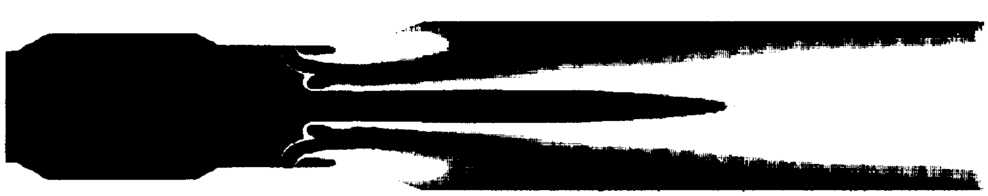

Figure 14. Temperature Contours for Premixed, Prevaporized RQL Combustor.[16]

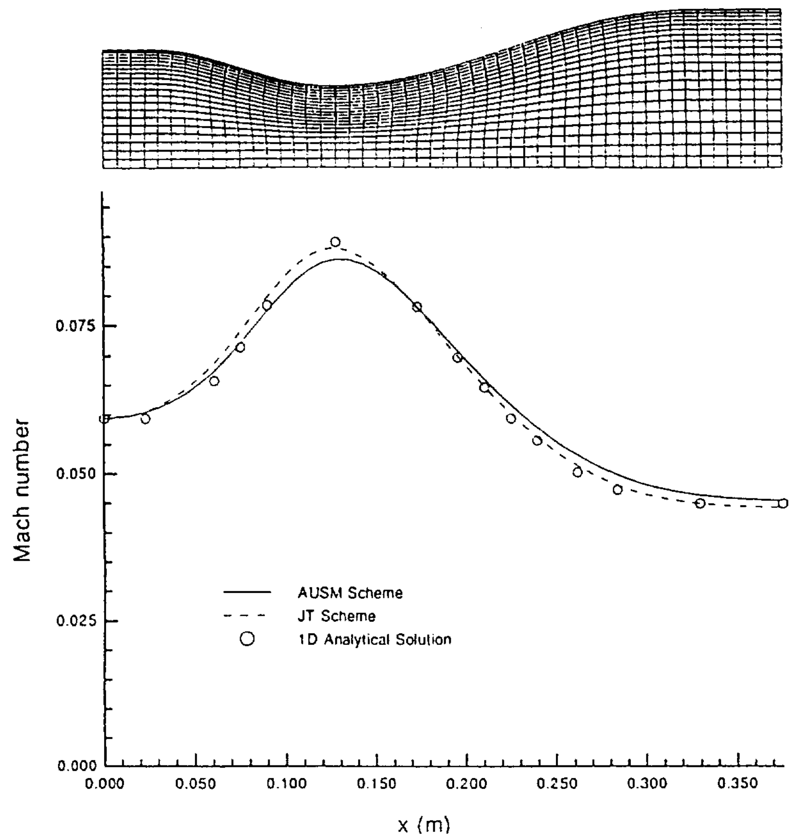

Figure 15. Comparison of LeRC-3D and Analytical Solution for Nozzle Flow.[3]